Preparation of pseudo-pure states by line-selective pulses in Nuclear Magnetic Resonance *

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Abstract

A new method of preparing the pseudo-pure state of a spin system for quantum computation in liquid nuclear magnetic resonance (NMR) was put forward and demonstrated experimentally. Applying appropriately connected line-selective pulses simultaneously and a field gradient pulse techniques we acquired straightforwardly all pseudo-pure states for two qubits in a single experiment much efficiently. The signal intensity with the pseudo-pure state prepared in this way is the same as that of temporal averaging. Our method is suitable for the system with arbitrary numbers of qubits. As an example of application, a highly structured search algorithm—-Hogg's algorithm was also performed on the pseudo-pure state $|\,00\rangle$ prepared by our method.

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I. INTRODUCTION

Quantum computers [1-4] use the principle of quantum mechanics and have been proved to have more advantages over classical computers. Quantum computation can be divided into three stages consisting of the preparation of initial states, computation, and the readout of the final states. The proper preparation of a fiducial pure state as inputs is an important part in the process. It is not only the starting point of the quantum computation, but also the foundation of quantum error correction [5-8]. In liquid-state NMR ensemble quantum computers [9], pseudo-pure states, the highly mixed states, provide a faithful representation for the transformations of pure states. Hitherto, several methods [9-16] have been proposed to prepare the pseudo-pure states including spatial averaging [9,10], temporal averaging [11], logical labeling [12,13,16], spatially encoding [14] and the cat-state benchmark [15]. In this paper, we report the experimental implementation of a new spatial averaging method for pseudo-pure state preparation with line-selective pulses and a field gradient pulse. We excite specific single-quantum transitions using selective pulses with appropriate rotating angles to equalize the populations of the energy levels expect an undisturbed one. Then a magnetic field gradient pulse along the *z-axis* is exploited to annihilate all transverse magnetizations caused by line-selective pulses. Possibilities of extending this preparation scheme to more than two-qubit system are discussed. Advantages and disadvantages of the scheme are analyzed. A practical example using the pseudo-pure state prepared with this method for a quantum algorithm is also presented.

II. NEW METHOD OF PREPARATION OF PSEUDO-PURE STATES

Consider a system with two spin-1/2 nuclei (AX) with energy levels labeled as Fig.1. In order to prepare a pseudo-pure state $\mid 00\rangle$, two single-quantum transitions irrelevant to the state, that is, the transitions $\mid 10\rangle \leftrightarrow \mid 11\rangle$ for spin X with the pulse angle β_1 and $\mid 11\rangle \leftrightarrow \mid 01\rangle$ for spin A with β_2 are excited simultaneously. The excitation yields the operator U [18],

$$U = exp(-i(\beta_1 I_x^{(3,4)} + \beta_2^{(4,2)} I)) \tag{1}$$

where $I_x^{(3,4)} = E_-^1 I_x^2$, $I_x^{(4,2)} = I_x^1 E_-^2$ and $[I_x^{(3,4)}, I_x^{(4,2)}] \neq 0$. Here, $I_\eta^i(\eta = x, y, z)$ are Pauli matrices of the *i-th* spin, and $E_\pm^i = \frac{1}{2}(1_2 \pm 2I_z^i)$. The superscripts 1 and 2 stand for the spins A and X respectively. $I_\eta^{(m,n)}$ are *Cartesian* single-transition operators, with *m,n* indicating the energy levels. Simultaneous excitation of two connected transitions is not straightforward to analyze, but modern computers supply software for manipulating this operation. In NMR, any pulse excitation corresponds to a unitary transformation, which can be written into the matrix form. We choose appropriate values of β_1 and β_2 through computer simulation to equalize the populations of the levels 2, 3 and 4. After applying a field gradient pulse *Gz* along the *z-axis* to annihilate all transverse magnetizations, the pseudo-pure state $|00\rangle$ is finally obtained. The pulse sequence of operations is

$$(\beta_1)_x(\beta_2)_x \rightarrow Gz \tag{2}$$

To make it more concrete, we shall show how to find out appropriate β_1 and β_2 for some specific quantum systems. Firstly, let us consider a homonuclear two-spin system, in which the gyromagnetic ratio γ_i of two spins is the same, namely $\gamma_1 = \gamma_2 = \gamma$. The deviation density matrix of the system in thermal equilibrium is

$$diag[eq] = [2, 0, 0, -2] \tag{3}$$

where "*diag*" represents the diagonal elements of the matrix and the common factor $\frac{\hbar B\gamma}{2kT}$ is omitted. After the application of the operator U to Eq.(3), the density matrix will evolve to

$$\rho_t = U\rho_{eq}U^+ \tag{4}$$

In order to get the pseudo-pure state, the following equations

$$\begin{aligned} \rho_t(2,2) &= \rho_t(3,3) \\ \rho_t(2,2) &= \rho_t(4,4) \end{aligned} \tag{5}$$

should be satisfied. Here, $\rho_t(n,n)$ indicates the -th diagonal element of the density matrix ρ_t. Solving Eq. (5), we get a set of appropriate solutions (β_1, β_2) in the range of $(0, 360^\circ)$, $(\beta_1, \beta_2) \approx (77.40^\circ, 77.40^\circ)$. Therefore, applying the pulse sequence of Eq. (2) to Eq. (3) leads to

$$diag[\rho_{eff}] = [2, -0.6667, -0.6667, -0.6667] = -0.6667 diag[E] + 2.6667[1, 0, 0, 0] \quad (6)$$

where E is a 4×4 unit matrix. It can be seen from Eq. (6) that, apart from a constant, is actually the pure state $|00\rangle$. For a heteronuclear two-spin system (i.e. $\gamma_1 \neq \gamma_2$) with ^{13}C and ^{1}H, the gyromagnetic ratio γ_1 is 1.4048 for ^{13}C and γ_2 is 5.5857 for ^{1}H. The deviation density matrix in thermal equilibrium is

$$diag[\rho_{eq}] = [6.9905, -4.1809, 4.1809, -6.9905] \quad (7)$$

where the common factor $\frac{\hbar B}{2kT}$ is also omitted. Applying the same procedures as the homonuclear system to Eq. (7), we get a set of solutions $(\beta_1, \beta_2) \approx (127.13^\circ, 186.01^\circ)$. The application of the pulse sequence of Eq. (2) yields finally

$$diag[\rho_{eff}] = [6.9905, -2.3303, -2.3303, -2.3299] = -2.3303 diag[E] + 9.3208[1, 0, 0, 0] \quad (8)$$

Three other pseudo-pure states$|01\rangle$,$|10\rangle$ and $|11\rangle$ for two-qubit system can be prepared with the similar procedures. The selective transitions and calculated pulse angles for preparing those states are listed in Table 1 along with those for $|00\rangle$ state.

Table 1 Parameters for pseudo-pure state preparation with selective pulses

pseudo-pure states prepared	Selective transitions		Pulses angles	
	Spin A (^{13}C)	Spin X (^1H)	β_1	β_2
$\mid 00\rangle$	$\mid 01\rangle \leftrightarrow \mid 11\rangle$	$\mid 11\rangle \leftrightarrow \mid 10\rangle$	127.13^o	186.01^o
$\mid 01\rangle$	$\mid 00\rangle \leftrightarrow \mid 10\rangle$	$\mid 10\rangle \leftrightarrow \mid 11\rangle$	127.13^o	186.01^o
$\mid 10\rangle$	$\mid 11\rangle \leftrightarrow \mid 01\rangle$	$\mid 01\rangle \leftrightarrow \mid 00\rangle$	127.13^o	186.01^o
$\mid 11\rangle$	$\mid 10\rangle \leftrightarrow \mid 00\rangle$	$\mid 00\rangle \leftrightarrow \mid 01\rangle$	127.13^o	186.01^o

The method outlined above can be, in principle, applied to systems with more than two qubits. For a three-qubit system with energy levels labeled in Fig.5. a route to cascade the other energy levels except the $|000\rangle$ one, $|\ 010\rangle \overset{1}{\longleftrightarrow} |\ 110\rangle \overset{2}{\longleftrightarrow} |\ 100\rangle \overset{3}{\longleftrightarrow} |\ 101\rangle \overset{4}{\longleftrightarrow} |\ 111\rangle \overset{5}{\longleftrightarrow} |\ 011\rangle \overset{6}{\longleftrightarrow} |\ 001\rangle$ can be utilized to apply simultaneously selective pulses. The pulse angles $(\beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \beta_6)$ exciting the corresponding transitions labeled by the numbers on the symbol are determined by equalizing the populations of all the levels involved. For a homonuclear system, they were calculated to be $(\beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \beta_6) \approx (182.02°, 179.04°, 229.38°, 193.46°, 200.28°, 105.75°)$. For a specific heteronuclear system consisting of the ^{13}C, ^{13}C and ^{1}H, calculation resulted to $(\beta_1, \beta_2, \beta_3, \beta_4, \beta_5, \beta_6) \approx (201.89°, 258.83°, 313.40°, 346.31°, 295.37°, 234.18°)$. A pseudo-pure state for a three-qubit system is thus achieved after a field gradient pulse is applied. If one could execute specific pectinate pulses and control their excitation intensity as required by developing NMR experimental technique and the instrumental function, the method can be extended to many-qubit systems.

III. EXPERIMENTAL NMR RESULTS

The scheme stated above was implemented by liquid-state NMR spectroscopy with carbon-13 labeled chloroform $^{13}CHCl_3$ (Cambridge Isotope Laboratories, Inc.). We chose H and C as the two-spin system in the experiments. Spectra were recorded on a Bruker-ARX500 spectrometer with a probe tuned at 125.77MHz for ^{13}C (denoted by A), and at 500.13MHz for the ^{1}H(denoted by X). The spin-spin coupling constant J between ^{13}C and ^{1}H is 214.95Hz. The relaxation times were measured to be T1=4.8sec and T2=0.2sec for the proton, and T1=17.2sec and T2=0.35sec for carbon nuclei.

The $|00\rangle$ pseudo-pure state was firstly prepared in the experiment. Selective excitations were executed using low-power, long-duration pulses of a *guass1k* shape. The length of these pulses was tailored to achieve sufficient selectivity in the frequency domain without disturbing the nearest line, depending on the magnitude of the J coupling constant. We

took all the length of the selective pulses to be 32ms in order to meet the requirement of simultaneity. The excitation powers for the channels ^{13}C and ^{1}H were set to be 56.7dB and 63.1dB so that the rotating angles of and were obtained respectively. The magnetic field gradient pulse was accomplished with the *sine-0* shape along the z axis. The spectra then recorded (shown in Fig.2) confirm that a pseudo-pure state $|00\rangle\langle 00|$ has been prepared. Fig.3 (a) and (b) show respectively the real and imaginary components of the deviation matrix of for the $|00\rangle$ state by quantum state tomography. The pseudo-pure state we obtained was

$$\rho = \begin{bmatrix} 1 & -0.0096 - 0.0090i & 0.0017 - 0.0026i & -0.0005 + 0.0006i \\ -0.0096 + 0.0090i & 0.0230 & -0.0020 + 0.0014i & 0.0033 + 0i \\ 0.0017 + 0.0026i & -0.0020 - 0.0014i & 0.0161 & 0.0095 + 0.0090i \\ -0.0005 - 0.0006i & 0.0033 - 0i & 0.0095 - 0.0090i & 0 \end{bmatrix}$$

The maximal relative error of the experimental values of the density matrix elements was <3%.Applying the corresponding transition-selective pulses given in Table 1 we got all the other pseudo-pure states $|01\rangle$, $|10\rangle$ and $|11\rangle$ for the two-spin system. The experimental results are shown in Fig.3.(c)-(h) with the maximal experimental error <5%.

IV. AN APPLICATION TO HOGG ALGORITHM

We experimentally implemented the Hogg's algorithm [19,20] with the pseudo-pure state $|00\rangle$ we prepared above. For a two-qubit system, the solution to the 1-SAT problem with two clauses was to be sought after. The logic formula is$V_1 \bigwedge V_2$, (V_1, V_2 are the logic variables). The corresponding solution is theoretically found to be $|11\rangle$. Applying the sequence in [20] to the pseudo-pure state $|00\rangle$, we got the results shown in Fig.4 with the experimental errors <5%.

V. DISCUSSIONS

In comparison with previous methods for preparing pseudo-pure states, the present method using line-selective excitations seems to be simpler and experimentally more efficient,. With temporal averaging [11], the preparation of a two-spin pseudo-pure state needs to carry out three different experiments. For spatial averaging proposed in [4], the magnetization are greatly lost due to the repeated magnetic field gradient pulses introduced in the course of the preparation so that the signal intensity is reduced. Moreover, as logical labeling[12,13,16] requires some qubits as ancillary bits, which don't participate in computation, much memory room is wasted. Furthermore its Signal-to-Noise ratio(SNR) is not ideal due to SNR$\propto nvN\alpha/2^N$ [12], with n being the molecular density of the sample, v the volume, and N the spin numbers of the sample molecule. In contrast, using the present method, one can apply fewer pulses to prepare a pseudo-pure state in a single experiment with the signal intensity of $\frac{2}{3}(\gamma_1+\gamma_2)$, the same as that of temporal averaging. Moreover, all pseudo-pure states for a specific spin system can be obtained with a judicious choice of line-selective pulses. Besides the errors due to the inhomogeneity of RF fields and static magnetic fields as well as imperfections of the pulse-length calibration, another main error in experiments is introduced from the imperfections of the line-selective pulses. Selective excitation of a *guass1k* shape leads to a large phase gradient of lines in excitation band. Theoretically, the phase gradient can be corrected in some way, but much base-line distortion will practically be caused. However, from the experimental results, we can find that the errors caused by the present method is smaller than that by previous ones. A difficulty of the present method is related to the sample choice. As line-selective pulses require all lines to be well-resolved, the coupling constants J should increase rapidly with the increase of the qubit number, but are still much smaller than chemical shift. It may be very hard to find out or synthesize such a sample for many-qubit system.

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Captions of the figures

Figure 1 The energy levels of a two-spin system (each with spin-$\frac{1}{2}$) and the scheme of preparing the pseudo-pure state $|00\rangle$.

Figure 2 Spectra of the prepared pseudo-pure state $|00\rangle$. The left indicates the spectra of ^{13}C and the right, ^{1}H. The reading-out pulses (a) , (b) and (c) were applied respectively. The abscissa indicates the frequency, and the ordinate denotes the intensity of the spectra (in arbitrary unit).

Figure 3 Experimentally measured deviation density matrices for the pseudo-pure states, denoting the $|00\rangle$,$|01\rangle$,$|10\rangle$and $|11\rangle$ states respectively from top to bottom. The left and right column show the real and imaginary components of those $|00\rangle$,$|01\rangle$,$|10\rangle$and $|11\rangle$ states respectively.

Figure 4 Experimental results of the final density matrix after implementation of the Hogg's algorithm of logical formula $V_1 \bigwedge V_2$ on the pseudo-pure state $|00\rangle$. (a) the real components. (b) the imaginary components.

Figure 5 The energy levels of a three-spin system (each with spin-$\frac{1}{2}$) and the scheme of preparing the pseudo-pure state $|000\rangle$.

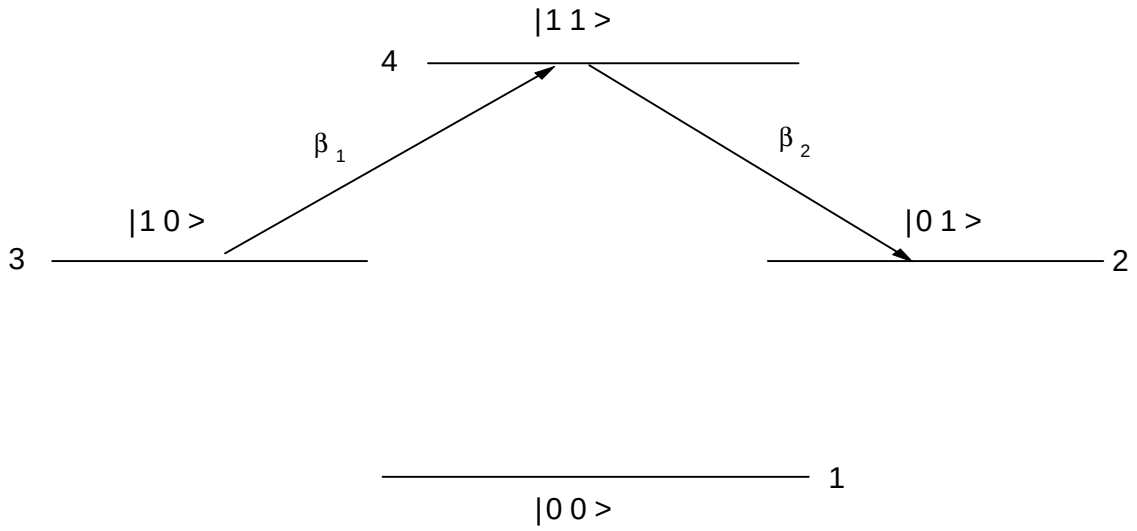

Fig. 1

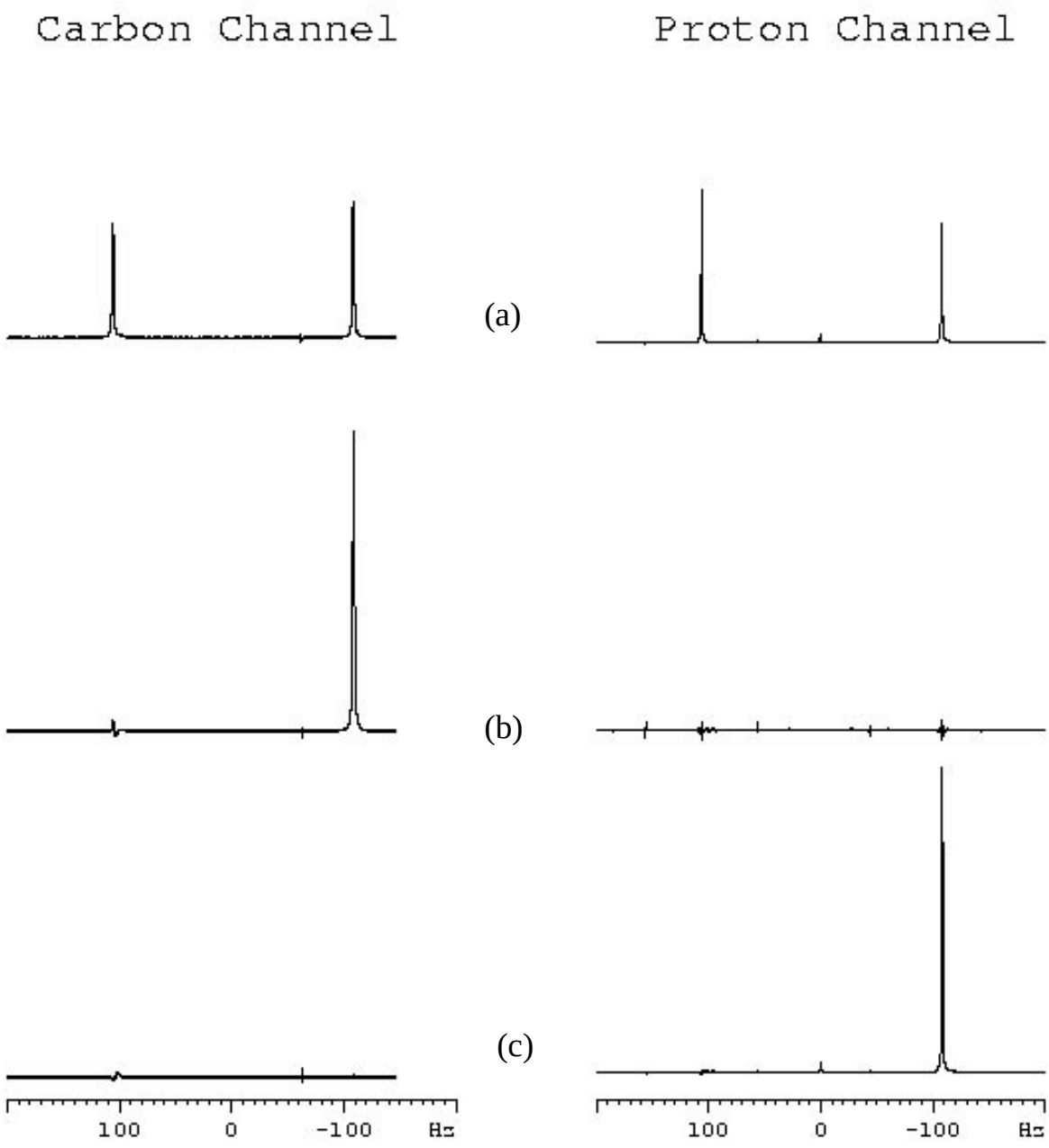

Fig. 2

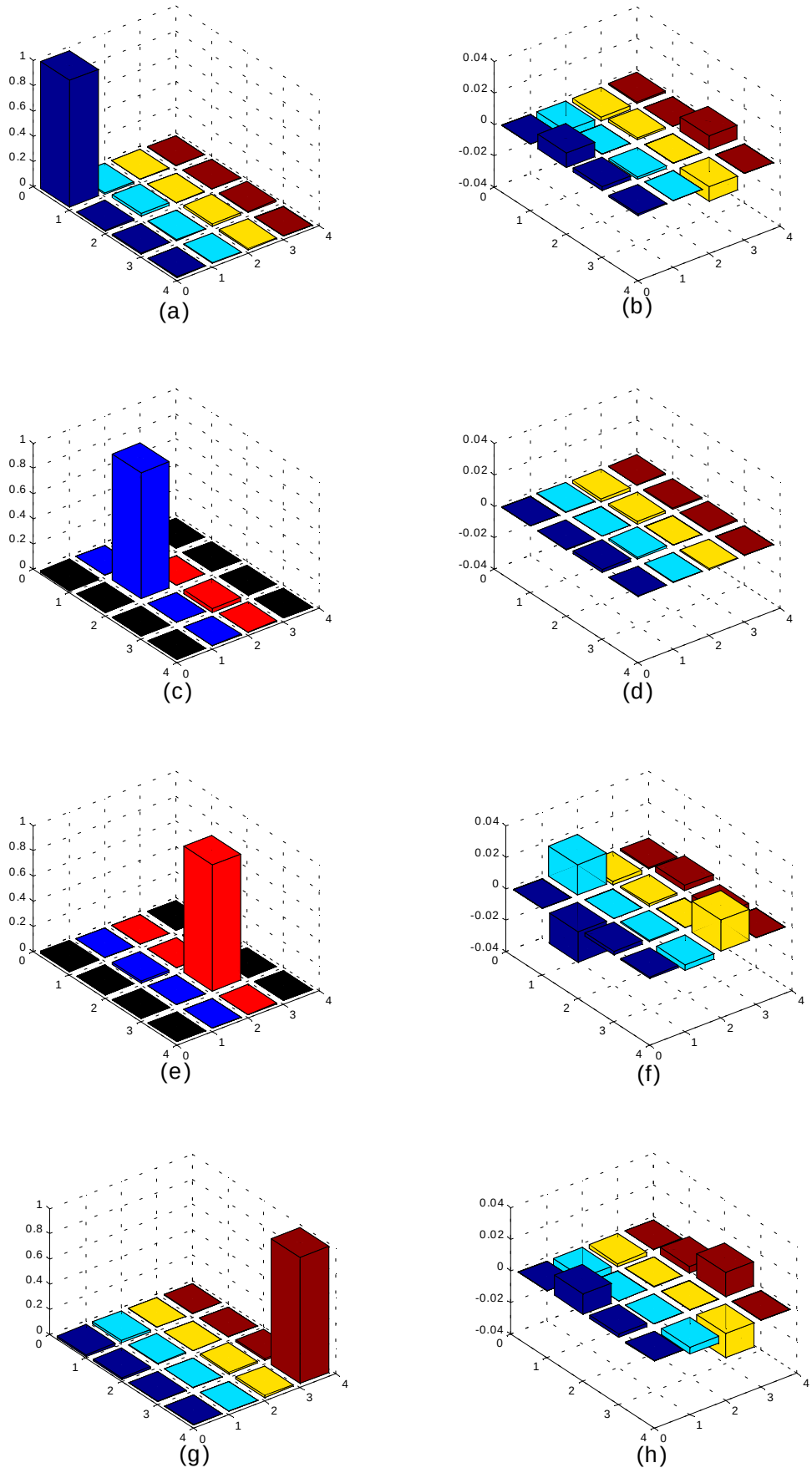

Fig. 3

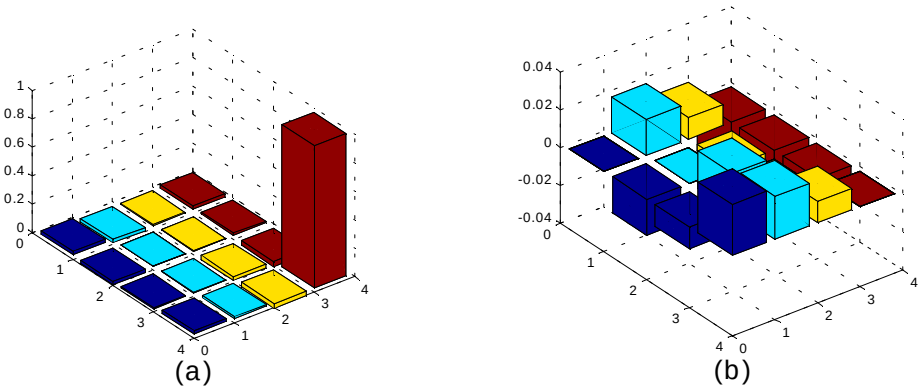

Fig. 4

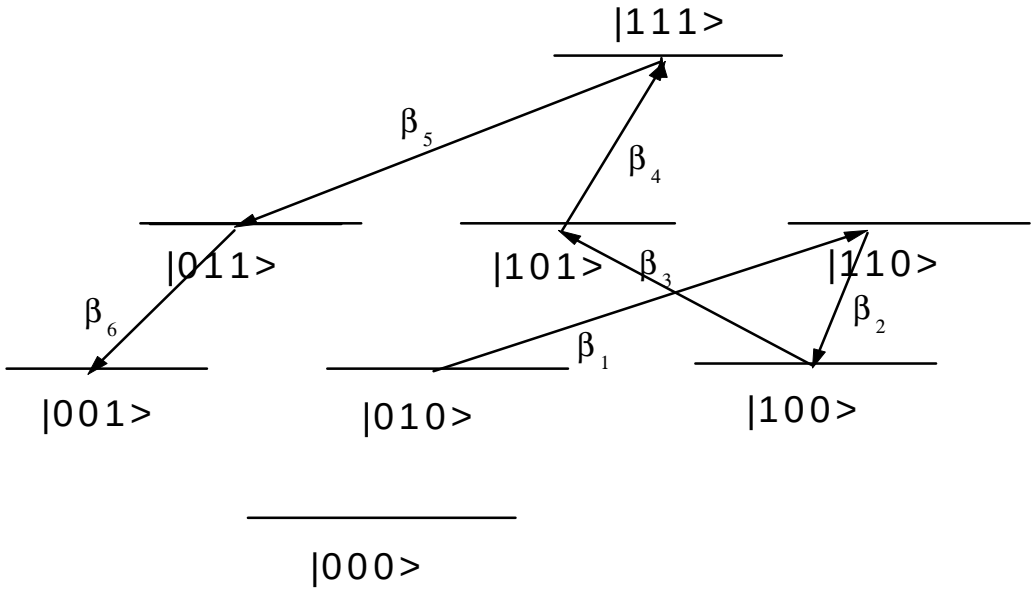

Fig. 5